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Environmental performance assessment of the chemical industries involved in the Responsible Care®Program: Case study of the Russian Federation

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ABSTRACT

The chemical industry is one of the typical sources of harmful pollutants and some of which are difficult to tackle. Sustainable Development Goals (SDGs) are of great concern to the performance of chemical industries regarding environmental impacts, and one of the core programs is the global voluntary Responsible Care® Program (RCP), aiming to encourage the industries to voluntarily report environmental performance data. Due to the voluntary reporting system, the collected datasets are huge while often heterogeneous, which makes it difficult to analyse the performance and evaluate the difference before and after the launch of the program. Direct comparison of actual indicators may fail to provide an accurate estimation of the implementing efficiency of the RCP. In this study, an original algorithm is developed to analyse the environmental KPIs of chemical companies involved in the RCP, in order to investigate the efficiency of the program and provide insightful suggestions for further development of the data reporting, as well as to provide advice for the further application of the program. The results showed that most of the environmental impacts of the chemical industries in the RF, e.g. soil pollution and water pollution, has been decreasing after the launching of the program. However, for both the companies involved in the RCP and the entire chemical industrial sector of the RF chemical industry, the GHG emissions maintained an increase. A major insightful conclusion is more energy has been used for improving more direct environmental impact, while the attention for impacts with longer harm potential, e.g. GHG emissions, has been shifted. Further policies and regulations should be targeted at the impact of the chemical industry on climate change, and new technologies should be encouraged to improve the efficiency of energy use and thus decrease GHG emissions.

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1. Introduction

The urgent need for quantifying and minimising the impact of chemical enterprises on the environment is reflected by Sustainable Development Goals (SDGs) approved by the UN (UN, 2014) – Goal 12, "Ensure sustainable consumption and production patterns", and Goal 13 "Take urgent action to combat climate change and its impacts", which were adopted in 2015. These goals are of great concern to the chemical industries since pollution from chemical industry is one of the key problems of a planetary scale. Responsible Care® Program (RCP) is organized by the International Council of Chemical Associations (ICCA), contributing to the Strategic Approach to International Chemicals Management (SAICM). The RCP was first launched in Canada in 1985 (Krantzberg et al., 2011). The aim of the program is to circumvent state-initiated excessive normative regulatory measures (Bélanger et al., 2009), and to generate a positive reputation in the community (Sandman, 2002) and maintain their social responsibility (Krantzberg and

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Theriault, 2017). Until 2016, it has been practiced in more than 65 countries around the world (ICCA, 2018a). Until the year 2019, there are more than 580 signatories joined the RCP Global Charter (ICCA, 2018a), which promotes by the 58 chemical manufacturers' associations around the world (ICCA, 2015b) and covers 96% of the world's largest chemical companies (ICCA, 2018a). This program has been recognized by the international community (including international organizations such as the UN) as the best sectoral initiative that fosters sustainability of chemical companies (ICCA, 2012) and as chemical industry contributions to the SDGs (ICCA, 2017). The RCP is also considered by many countries and organizations as the main tool for chemical plants to regulate their environmental impact (King and Lenox, 2000), and as a tool for stimulating the continuous refinement of the main indicators in production processes, environmental protection, health maintenance (Khair et al., 2018), and the assurance of safety and social responsibility (Bélanger et al., 2014). RCP has been promoted and supported in both global (Lee et al., 2014) and regional scales (APEC, 2011). For instance, China has joined the RCP community in 2014, and more than 4000 chemical enterprises signed in the program (BASF, 2015). India started to promote the RCP since 2006, and there are in total 125 industries are signatories to the programme until the beginning of 2018 (Indian Chemical Council, 2018).

But SDGs are not only useful for the minimization of chemicals pollution; Impact on climate is also very important for the entire chemical industrial sector. Since mitigating global warming is one of the SDGs of the UN (UN, 2014), climate change, particularly caused by GHG emissions, is also a global problem (Rockström et al., 2009) and plays an important role in human life (Minx et al., 2013). Carbon footprint and the more comprehensive GHG footprint, have been widely discussed by academia, media, and the public (Finkbeiner, 2009). It is found that chemical companies bear some responsibility for the increasing GHG emissions, including CO_2, NOx, methane, and fluoro hydrocarbons (Klemeš et al., 2016). To mitigate the climate changes, efforts have been made on reducing direct GHG emissions and increasing carbon captures (Arias et al., 2016), as well as indirectly improving management of major emitters. Climate change, along with the goals of sustainable production and consumption, is one of the subjects of the RCP to regulate chemical industries reducing their environmental performance. In the document "The SAICM Journey: 20 Milestones to 2020" devoted to the achievements of the RCP was noted that global chemical industry had improved their environmental performance (ICCA, 2018b). Since the year 2006, companies involved in the RCP have reduced GHG emissions by 34% (ICCA, 2018a), even though the number of reporting regions has doubled. The involvement of automotive building construction and light industries in the RCP have also facilitated a combined GHG emissions reduction of 3 Gt/y of (ICCA, 2015a).

In Russia, a national report was published in 2016 on the inventory of anthropogenic emissions by sources and removals by sinks of GHGs that are not regulated by the 1990–2014 Montreal Protocol. The report is consistent with the Intergovernmental Panel on Climate Change (IPCC) Guidelines (IPCC, 2007) and identifies four categories of general emission sources: energy, industrial processes and use of products, agriculture, and waste (Nakhutin et al., 2016). The largest contributor to GHG emissions in Russia in the energy sector is fuel combustion (65.1% of total GHG emissions in the year 2014 accounted). The most significant source of emissions in the industrial sector is metallurgy (41.8% of the total industrial GHG emissions in 2014). In the chemical sector, ammonia production and methanol production are known for the largest amount of GHG emissions.

Increasing interest in social and environmental issues has been a reason for implementing environmental activities as a part of a voluntary corporate strategy in industries (Despeisse et al., 2012). In some papers RCP is described as an example of successful voluntary commitment by the global chemical industries (West, 2007), to drive continuous improvement and achieve excellence in environmental, health, safety and security performance. The previous studies (Finger and Gamper-Rabindran, 2011) showed that the occurrence of incidents considerably decreased in companies that are involved in the program. In addition, studies also showed that the program has favoured a considerable decrease in environmental impacts (Moffet et al., 2004) from its beginning. However, some authors had doubts regarding the effectiveness of the RCP as a tool for the chemical industries to minimise the environmental impact (Gamper-Rabindran and Finger, 2013). Consequently, there is a need for the development of an approach to the unambiguous interpretation of the achievements of the chemical industries, which is important for the estimation of how RCP promoting the SDGs.

The use of indicators for the environmental impact assessment (Schreiber et al., 2016) is common practice in the analysis of the state of complex systems (Klemeš, 2015). Some indicators are used for global assessments of ecological (Čuček et al., 2012) and GHG including CO_2 footprints (Klemeš et al., 2016). The GHG footprint is calculated as the aggregate of GHG emissions directly or indirectly produced by a person, organization, region, related to the performance of an activity, provision of a service and production of products, during the lifecycle of the object (Gombiner, 2011). It is measured in equivalent CO_2 t/y and calculated as the mass of a given GHG multiplied by its global warming potential (GWP) (Muthu, 2016). A recent review of GHG emission footprint (Hickmann, 2017) revealed that methods for estimating the GHG footprint of products are based on standards, methodological guidelines, and adopted sectoral schemes and programs (Gao et al., 2014). However, they are also used in relation to the technological advances of the specific production process (Klemeš and Varbanov, 2013). Among these are GHG Protocol Product Standard, PAS 2050: 2011, Guidelines for National GHG Inventory of the Intergovernmental Panel on Climate Change (IPCC, 2007), and ISO 14047 (International Organization for Standardization, 2012) etc. A number of approaches allow the estimation of GHG emissions via several approximations to differ in the scope of coverage (Ranganathan et al., 2004). To assess the rate of climate change and reduce GHG emissions, the world's largest companies provide voluntary reporting under the global Carbon Disclosure Project (CDP) initiative (Hassan et al., 2013). It should be noted that despite the various methods, there is currently no globally unified approach to assessing GHG footprints (Scipioni et al., 2012), especially methods dealing with incomplete data. Companies participating in the RCP also provide data on GHG emissions for the reporting period.

Various Key Performance Indicators (KPIs) have been also used to quantitatively assess the efficiency of RCP implementation in the field of environmental protection of chemical companies (ICCA, 2015a). To date, an enormous amount of data on these KPIs has been collected for the period from 2000 until 2016 during the implementation of the RCP. Some countries use KPIs for the assessment of efficiency and sustainability in the chemical industry (Barbosa and Gomes, 2015). The collected datasets are huge and often heterogeneous, which makes it difficult to analyse information (Makarova et al., 2017). For example, according to the studies of ICCA (2015a), an analysis of collected data, including those on the total chemical oxygen demand (COD) and emissions of sulphur dioxide (SO_2) and nitrogen oxides (NOx) provided in the ICCA 2015 report (ICCA, 2015a). The report traced the trends and indicated that with the increase of reporting companies. The total CO_2

emissions increased from 2000 to 2013, but the CO_2 intensity, calculated as the total CO_2 emission divide by the total amount of products, has been decreasing obviously. The decrease indicates the improvement of energy use as is shown in Fig. 1.

The contribution of this work is to evaluate the performance of RCP as a tool for the chemical industry to fulfil the SDGs regarding environmental issues. The study would provide benchmarking values for the program managers to better improve the program performance. The result would also help the involved industries to seek potential directions in reducing environmental impacts of the chemical industries.

The aim of this study is estimation how RCP promotive of SDGs. Upon entering the program, enterprises commit themselves to annually providing comprehensive data on the environmental impact and industrial safety. Since the direct comparison of actual indicators may fail to provide an accurate estimation of the implementing efficiency of the RCP, an original algorithm has been developed in this study to analyse the environmental KPIs of chemical companies involved in the RCP. The KPIs for analysis are obtained from the chemical plants of the Russian Federation over a period of 11 y; which makes it possible to better estimate the energy efficiency of the RCP and perform a systematic analysis of various activities of the companies. Major novelties of this work are 1) the proposed Heuristic Approximation Algorithm dealing with the data incompletion issue. 2) Assessing the environmental performance of the industries involved in the Responsible Care Program in the Russian Federation and provide insightful suggestions for the further improvement of the voluntary participation of the industries to reduce environmental impacts.

2. Subjects of the study

The subject of the study covers the abundant dataset of environmental impact assessment indicators of chemical companies in the Russian Federation collected during an 11-year period. It should be noted that the RCP is rather flexible (Fransen and Conzelmann, 2015), which allows one to adapt the program considering country specifics (Moffet et al., 2004) and results in certain differences in the number of indicators collected in various regions and countries. The data analysed in this paper are the reported annual indicators (separately by companies) relating to the impact on environmental subsystems:

1) Solid waste to be disposed of: the amount of hazardous and non-hazardous waste expressed in t.
2) Atmospheric pollution: SO_2, volatile organic compounds (VOC), NOx, carbon oxide (CO) expressed in t.
3) Estimation of the impact of climate change was estimated on the basis of emissions of GHGs, including CO_2, NOx, hydrofluorocarbons (HFCs), and methane (CH_4), expressed in CO_{2eq}.
4) Water pollution: COD, and the amount of phosphorus-containing and nitrogen-containing compounds, and the total amount of discharged hazardous chemical compounds expressed in t. Amount of consumed and discharged water expressed in m^3.
5) Indicators of energy and resource consumption: data of the electric power in W/h, heat in kcal, and fuel consumption, e.g. natural gas in m^3.
6) Expenses on environment protection measures, expressed in RUB.
7) Total production of chemicals expressed in t.

These indicators were chosen because they are the main KPIs within the RCP program and possessed better data availability. The reporting of these indicators has been conducted since 2005.

In this paper, linear extrapolation is used to extrapolate the data received from the RCP database. Based on the proposed approach, this study assessed the efficiency of voluntary initiatives, following the example of the Russian Federation chemical companies under RCP and the possibility of extrapolating these estimates to the entire chemical industry.

The algorithm developed in this paper allows us to assess the implementation efficiency of the RCP regarding emission reduction, including waste, SO_2, NOx, VOC, CO, GHG (the approximations 1 and 2 at the World Resources Institute recommendations (World Resources Institute, 2001) are estimated), COD, discharge of phosphorus-containing and nitrogen-containing chemical compounds, etc. The GHG emissions data is not widely available from RF companies because it is not required in official reporting, and thus is difficult to calculate the absolute GHG emissions from Russian Federation chemical industries. The analysis of information from companies involved in the RCP might give us the opportunity to understand trends in the RF.

3. Methods

3.1. Data source

At the end of 2015, over 60 Russian Federation companies signed the agreement on the RCP and provided the according to reports. The original dataset used in this study on KPI statements of the Russian Federation chemical companies under RCP is available in the RCP database (see Appendix 1). The processed data used in this study is shown in the supplementary attachments. In total, the

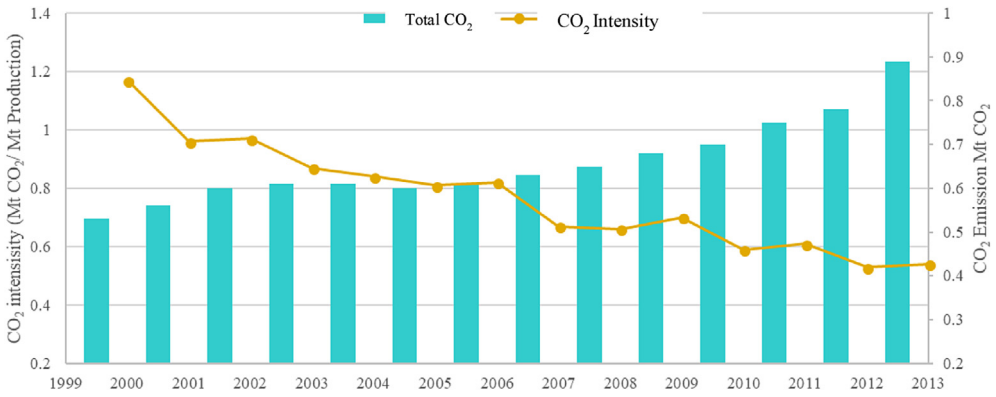


Fig. 1. CO_2 emission and CO_2 intensity reported by companies involved in the RCP.

companies have provided the reports of about one-third of all chemical products of the RF, which enables the analysis of the obtained industries and estimation of the entire chemical industry of the RF. The validity of this approach may be partially justified by the study (Lenox and Nash, 2003), according to which, the more significant a company's impact on the environment, the more it is inclined to join various ecological initiatives, such as the RCP.

The input data of the case study includes: the amount of pollutants from chemical industries involved in the RCP, including Solid waste (hazardous and non-hazardous); Atmospheric pollutants (SO_2, VOC, NOx, CO); GHG emissions (CO_2, NOx, HFCs, and CH_4, Water pollutant (Water consumption and discharge, COD, phosphorus-/nitrogen-containing compounds, and discharged hazardous chemical compounds); Energy consumption (Electricity, heat, natural gas consumption).

3.2. Heuristic approximation algorithm

A heuristic approximation algorithm has been developed to perform the system analysis of estimates on the efficiency of environmental activities of chemical companies. An algorithm that includes several different assessment approaches were used to improve the accuracy of the findings obtained in the case of gaps in the data:

1) The dynamics and trends for absolute parameters are estimated;
2) The results obtained with the dynamics in relative indices (t/kRUB and t/t product) are compared;
3) The estimation of the entire chemical industry of the Russian Federation.
4) The results of individual companies (where possible and present more than 35% of the required data) are exported and the overall trend of the entire chemical industrial sector are estimated.

The coincidence of trends in three assessments gives us the opportunity to speak with confidence about the trend in the indicators. The positive or negative result of the environmental activities of chemical companies was estimated as well. The main stages and steps (see Fig. 2) of the heuristic approximation algorithm for the *i*th KPI are as follows:

Stage 1. Estimate the environmental impact assessment of *J* chemical companies (*J* is the number of companies) and foreign companies in some specific terms:

1.1) Calculate the aggregated absolute indicators i_a^n (where *n* is the reporting year) of the environmental impact assessment of *J* chemical companies that provided reports

$$i_a^{n,i} = \sum_{j=1}^{J} i_j^{n,i} \quad (1)$$

1.2) Determine the trends over an 11 y period of $i_a^{n,i}$ variation by years using the linear approximation procedure and least squares method.

Stage 2. Estimate the environmental impact assessment of *J* chemical companies in relatively specific terms.

2.1) Calculate the normalised or specific (i.e. V_m^n - t/t products, and/or in monetary terms $V_\$^n$ -*t/kRUB*) aggregated indicators $i_{norm}^{n,i}$ (where *n* is the reporting year) for the environmental impact assessment of *J* chemical company involved in the RCP that provided the reports:

$$i_{inorm,m}^{n,i} = i_a^{n,i} \Big/ V_m^n \quad (2)$$

$$i_{norm,\$}^{n,i} = i_a^{n,i} \Big/ V_\$^n \quad (3)$$

2.2) Determine the trends over an eleven-year period ($n = 1 \div 11$) of $i_{norm,m}^{n,i}$ and $i_{norm,\$}^{n,i}$ using linear approximation procedures and the least squares method;

Stage 3. On this stage have been used the approach to calculate the slope of the trend line via an original algorithm using data received from enterprises, with the gaps in the data being replenished using extrapolation and interpolation methods. It is assumed that this methodology can be applied to approximate the performance for Russian Federation chemical companies that provided reports, by using the indicator represented by the slope of the linear approximation resulting trendline drawn on the set of complex plots, an illustrating example is presented in Fig. 3.

It is assumed there are three companies voluntarily reporting their data, and the collected dataset is incomplete, as is shown in Fig. 3. The dark thin straight lines indicate the linear approximations of the KPI of each company, and the red straight line on the top can indicate the approximation of the overall KPI (covering the 3 companies). The estimation would improve the accuracy with data incompletion situations, such as the dataset from a voluntary reporting program in this study.

3.1) Calculate the E_j^i as the slope of the trend line of the KPI that is estimated and drawn onto a set of complex plots for the *j*th particular company. Calculate the E_j^i for all *J* chemical companies that provided reports for more than 4 y;
3.2) Calculate the performance parameter for the all chemical companies involved in the RCP for the KPI E_{mean}^i

$$E_{mean}^i = \sum_{j=1}^{J} E_j^i \quad (4)$$

Stage 4. Estimate of the entire chemical industry of the Russian Federation.

4.1) Extrapolate with using the normalised aggregated indicators $i_{norm,m}^{n,i}$ and $i_{norm,\$}^{n,i}$ and volume of manufactured products (in mass terms $V_{ind,m}^n$ and/or in monetary terms $V_{ind,\$}{}^n$) the result from companies involved in the RCP to the chemical industry of the Russian Federation in general:

$$i_{ind,m}^{n,i} = i_{norm,m}^{n,i} \times V_{ind,m}^n \quad (5)$$

$$i_{ind,\$}^{n,i} = i_{norm,\$}^{n,i} \times V_{ind,\$}^n \quad (6)$$

4.2) Determine the annual trends of $i_{ind}^{n,i}$ using linear approximation procedures and the least squares method.

Stage 5. Estimate the efficiency of environmental activities of a chemical company involved in the RCP. The efficiency of environmental activity of chemical companies is calculated over an eleven-year period for the entire industry via the parameter E_{total}

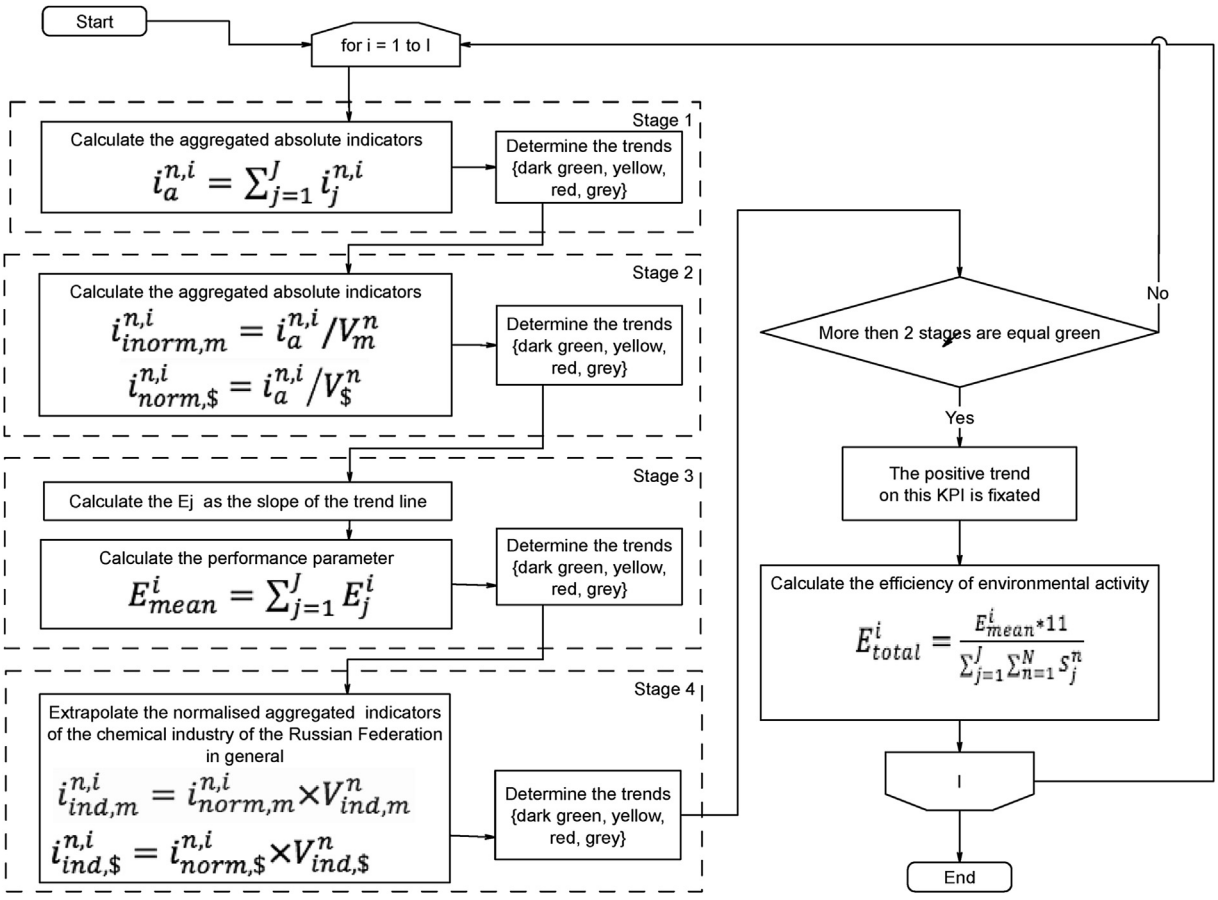
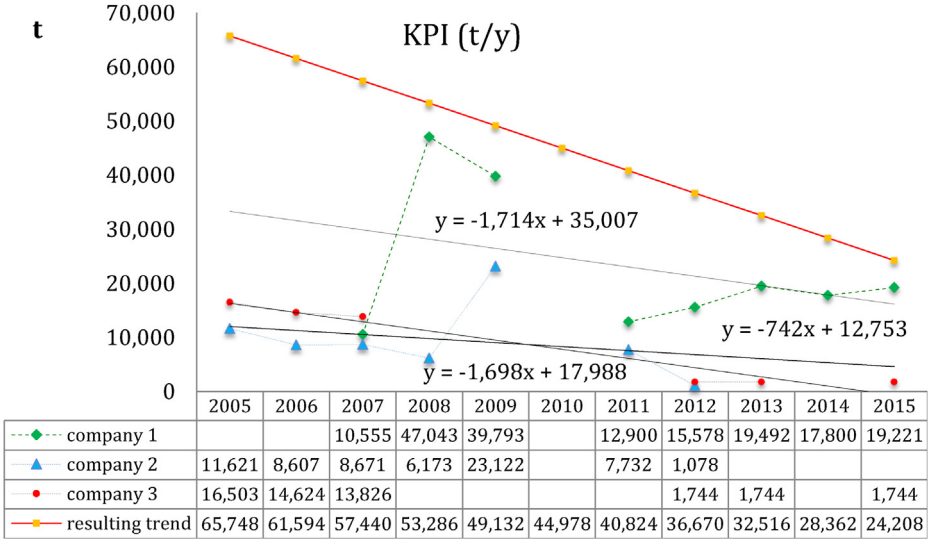

Start
for i = 1 to I
Stage 1
Calculate the aggregated absolute indicators
$i_a^{n,i} = \sum_{j=1}^{J} i_j^{n,i}$
Determine the trends {dark green, yellow, red, grey}
Stage 2
Calculate the aggregated absolute indicators
$i_{inorm,m}^{n,i} = i_a^{n,i}/V_m^n$
$i_{norm,\$}^{n,i} = i_a^{n,i}/V_\$^n$
Determine the trends {dark green, yellow, red, grey}
Stage 3
Calculate the Ej as the slope of the trend line
Calculate the performance parameter
$E_{mean}^i = \sum_{j=1}^{J} E_j^i$
Determine the trends {dark green, yellow, red, grey}
Stage 4
Extrapolate the normalised aggregated indicators of the chemical industry of the Russian Federation in general
$i_{ind,m}^{n,i} = i_{norm,m}^{n,i} \times V_{ind,m}^n$
$i_{ind,\$}^{n,i} = i_{norm,\$}^{n,i} \times V_{ind,\$}^n$
Determine the trends {dark green, yellow, red, grey}
More then 2 stages are equal green
No
Yes
The positive trend on this KPI is fixated
Calculate the efficiency of environmental activity
$E_{total}^i = \frac{E_{mean}^i * 11}{\sum_{j=1}^{J}\sum_{n=1}^{N} S_j^n}$
I
End

Fig. 2. The flowchart of the overall method.



	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015
company 1			10,555	47,043	39,793		12,900	15,578	19,492	17,800	19,221
company 2	11,621	8,607	8,671	6,173	23,122		7,732	1,078			
company 3	16,503	14,624	13,826					1,744	1,744		1,744
resulting trend	65,748	61,594	57,440	53,286	49,132	44,978	40,824	36,670	32,516	28,362	24,208

Fig. 3. Example of the RCP implementation trend based on an illustrating KPI (t/y).

$$E_{total}^i = E_{mean}^i * 11 \Big/ \sum_{j=1}^{J}\sum_{n=1}^{N} S_j^n \quad (7)$$

where S_j^n is the total environmental protection expense of the j^{th} particular company for the n^{th} year (alternatively, it can use $S_{atm,j}^n$, i.e. total atmospheric air protection expense of j^{th} particular company for the n^{th} year).

3.3. Indirect GHG emissions

In addition to direct GHG emissions, the indirect emission from

consumption of materials, energy, and heat at the enterprises can significantly influence the assessment. When calculating the GHG emissions, in terms of CO_2, the final report prepared by the European Bank for Reconstruction and Development (EBRD, 2010), was referenced to determine the GHG Emission Factors (EF_{GHG}). The overall EF_{GHG} for entire Russian Federation is listed in Table 1.

To transfer thermal energy, the following conversion is used: 1 Gcal (inter) = 1163 MW. Calculation of GHG emissions for natural gas for individual sources (furnaces) is calculated based on the approach in IPCC guideline (IPCC et al., 2006):

$$E = \frac{44}{12} \times M \times K_1 \times NCV \times K_2 \quad (8)$$

where: E - annual GHG emissions in weight units (t/y); M - actual fuel consumption for the year (t/y); K_1 - carbon oxidation factor of the fuel, fraction; NCV - net calorific value (J/t); K_2 – C emission factor (t/J); *44/12* - the conversion factor of C into CO_2 (molecular weights: C = 12 g/mol, O_2 = 32 g/mol, CO_2 = 44 g/mol). In this study, natural gas is considered as the major energy consumption, and the NCV of natural gas is 37.5 TJ/kt (IPCC et al., 2006). During fuel combustion, not all the comprising carbon is oxidized to CO_2, and incomplete combustion of fuel is taken into account via the K_1. The average value of K_1 for natural gas is 0.995 (IPCC et al., 2000). K_2 is set as 15.3 kt/TJ according to (IPCC et al., 2006).

The density of natural gas is from 0.68 to 0.85 kg/m^3 relative to the dry air. In the calculation, it is considered equal to 0.75 kg/m^3. Therefore Equation (8) can be processed as:

$$E = \frac{44}{12} \times V \times 0.75 \times 0.001 \times 0.995 \times 37.5 \times 15.3 = 1.43 \times V \quad (9)$$

Where V is the volume of natural gas, m^3.

4. Results

4.1. Soil pollution

The impact of chemical industries on soil pollution is estimated by using the indicators of the amount of hazardous and non-hazardous wastes deposited by the companies. The results of calculated on stages 1 (i_a) and 2 ($i_{norm,m}$, $i_{norm,s}$) of the heuristic approximation algorithm of the deposited amounts of hazardous and non-hazardous wastes by the chemical companies are shown in Fig. 4.

The analysis identified an insignificant increase in the amount of hazardous waste from Russian chemical companies during the period from 2005 to 2007 and 2008 to 2012. After 2012 the situation of the hazardous waste generation is stable (Fig. 4a), but the specific amount of hazardous waste (Fig. 4b and c) continuously decreases. Although the absolute amount of non-hazardous waste disposal increases (Fig. 4d), the specific disposal decreased tenfold from 15 t/t to 1.65 t/t during the 10 y of program implementation (Fig. 4e).

The indicator for the entire chemical industry does not show any considerable change in the estimates of chemical waste disposal. Extrapolation to the entire RF chemical industry also shows a decrease in the formation of non-hazardous waste from 803 Mt/y in 2007 to 275 Mt/y in 2013 (Makarova et al., 2018).

Table 1
EF_{GHG} of the RF in 2009–2016 (EBRD, 2010).

Year	2009	2010	2011	2012	2013	2013	2015	2016
tCO_2/MWh	0.617	0.616	0.624	0.642	0.632	0.629	0.640	0.632

4.2. Atmospheric pollution

The atmospheric pollution was estimated by considering the following types of atmospheric emissions: SO_2, NO_x, VOC and CO. The system analysis results for estimates of atmospheric emissions of the main pollutants calculated via a heuristic approximation algorithm (stages 1 and 2) presented in Fig. 5.

Atmospheric emissions of SO_2 and NO_X from RF chemical companies involved in the RCP increase in absolute amount (Fig. 5a and d) but decrease in relative indicators (Fig. 5b, e, 5c, and 5f). The absolute emissions of VOC decreased during the period from 2008 to 2010 before a considerable increase to 2012 and decreased after (Fig. 5g). However, the specific VOC emissions (Fig. 5h and i) shows no notable change afterwards in 2008. Both the absolute and relative emissions of CO increased (Fig. 5j and k and 5l), which is due to the ever-increasing number of chemical companies that began to monitor this parameter during this time.

Within the entire industrial sector (Fig. 5l), the emissions of SO_2, NOx, and VOC remained nearly unchanged after 2008, while for SO_2 and NO_X, a minor decrease can be observed from 2007 to 2013 (Makarova et al., 2018).

To assess the adequacy of the data received. The expected results, on the whole, were compared with the official statistics (Federal State Statistics Services, 2018). Fig. 6 shows the official statistics of the Russian Federation for some industries, which include certain types of chemical products. The trend lines for total emissions are identical to the trends for nitrogen and sulphur oxides, which account for the bulk of mass emissions for the period under review.

Conversely, the emissions of CO considerably increased during the studies period. The Russian Chemists Union, which represents the chemical company involved in the RCP, ranks 6th to 12th among all other associations that provide reports on SO_2 emissions, and 4th to 8th on NO_2 emissions. In terms of VOC emissions, RF companies are generally one of the three leading contributors, along with companies from France and Australia, to environmental pollution.

4.3. Impact on water systems

An estimation of the impact on water systems was performed using indicators such as COD, discharge of nitrogen-containing and phosphorus-containing chemical compounds, the total amount of discharged hazardous chemical compounds, and amount of consumed and discharged water.

The diagrams in Fig. 7 demonstrated the dynamics of changes in amounts of consumed and discharged water for the fast-growing industry that is to a large extent analogous to the dynamics of wastes disposal, where the absolute amount of wastes increases but the specific waste disposal (t/t product) decreased.

The amounts of discharged water increased from 2005 to 2010 and no clear dynamics is observed afterwards, and the specific water use (m^3/t product) showed a slight decrease during the study period, which indicates the improvement of water use efficiency. The water use in the entire chemical industrial sector also decreased.

The results of estimations on the efficiency of chemical companies in the protection of water systems are shown in Fig. 8. Estimation of the number of selected water pollutants of the chemical companies using the selected criteria expressed in absolute amounts does not reveal any clear dynamic trends. For example, the nitrogen-containing compounds showed an increase from 2005 to 2010 and a decrease from 2011 to 2014. However, a

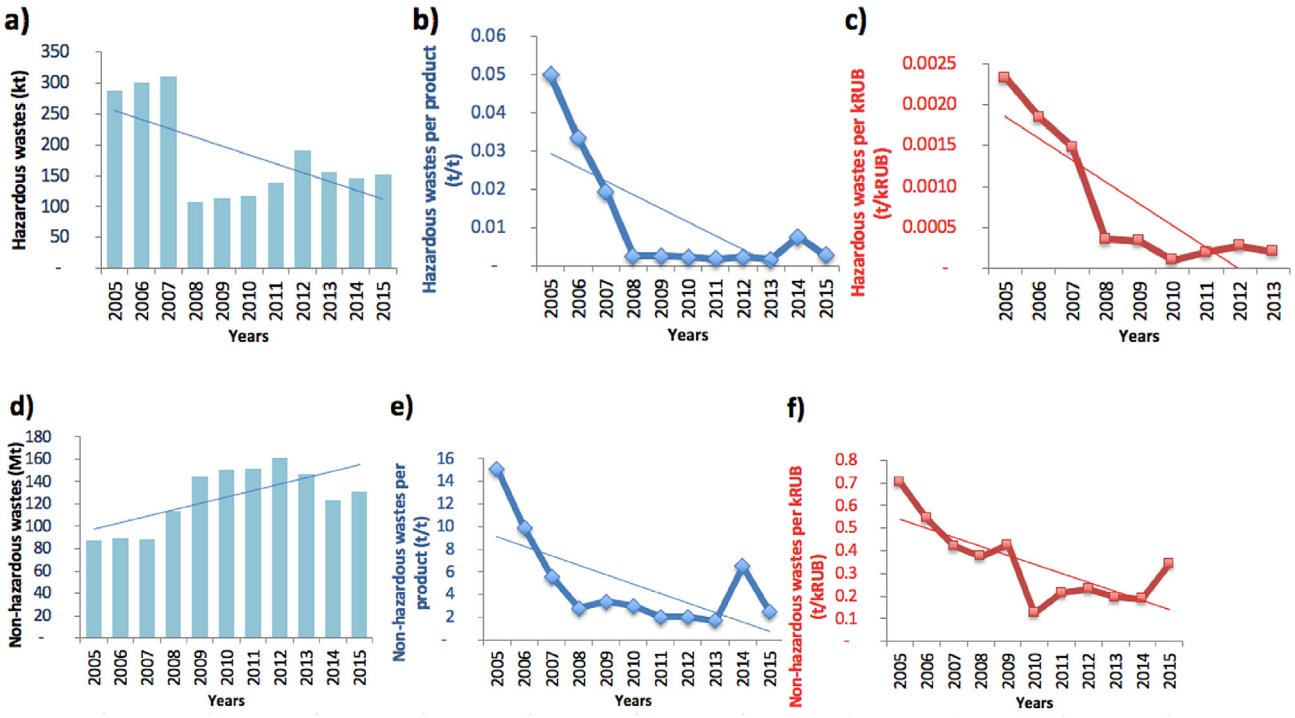


Fig. 4. Hazardous and Non-hazardous Waste disposal of the companies involved in the RCP: a) and d) absolute value (i_a, t); b) and e) disposal of unit product ($i_{norm,m}$, t/t product); c) and f) disposal of unit RUB ($i_{norm,\$}$, t/kRUB).

clear decrease in the specific values (t/t product and t/k RUB) are observed for all indicators. Additionally, a decrease of the selected water pollutants from the entire chemical industry is clearly observed for selected indicators expressed in absolute amounts.

4.4. Energy consumption

Data of the electric power, heat, and fuel consumption of both the RCP member companies and the entire chemical industrial sector are presented in Fig. 9.

Fig. 9 showed a pre-2008 decrease that precedes an increase in the absolute consumption of energy resources for the companies involved in the RCP in the RF, but with a decrease in the consumption per unit products. Such behaviour may be the result of government-supported energy and resource saving programs. Estimation of energy consumption by RF companies has shown that this parameter has increased in absolute and relative amounts from 2005 to 2015, whereas its stabilisation, or even a slight decrease for the entire chemical industrial sector.

4.5. Estimation of GHG emissions

The impact of chemical companies on climate change was estimated on the basis of emissions of GHGs, including direct CO_2 emission, NO_x, HFCs, and CH_4. To make an overall estimate of the contribution of emissions of chemical companies to the greenhouse effect, the GHG emissions are calculated as the CO_2 equivalent ($CO_{2\text{-}eq}$). The conversion coefficients were referred from IPCC report (IPCC, 2007) for the average effect exceeding 100 t/t. The GHG emissions are presented in Fig. 10.

The averaged estimates (both absolute and relative) of GHG footprints of the companies involved in the RCP are shown in Fig. 11.

5. Discussion

5.1. Analysing the environmental KPIs

To overview the changes of the environmental indicators during the implementation of RCP, the trends of the selected indicators covers the KPIs in the following aspects:

- **Soil pollution:** dangerous and not dangerous waste (after 2012)
- **Atmospheric pollution**: SO_2 (after 2009), NOx, CO, and VOC emissions
- **Water consumption and pollution**: water consumption and discharge (after 2013), COD and nitrogen/phosphorous-containing compounds
- **Energy consumption:** the consumption of major energy resources
- **Climate changes:** GHG emissions and footprints

Based on the diagrams in the results section, the changing trends were categorized into 4 types: Increase, Decrease, Stable, and No clear trends. The estimation results based on the data from all chemical industries involved in the RCP are presented in Table 2.

It is clear that during the implementation period of the RCP, the absolute value of the most of selected indicators increased or keep stable during the period, but the specific pollution or consumption (t/t product or t/kRUB) of most indicators decreased. It is worth noticing that during this time, the trend of energy consumption and GHG emissions and footprint are not clear.

The results based on the 11 y data showed positive trends for 9 KPIs (green in most cells in Table 2). And for 12 KPIs in relative indicators (t/t product or t/Krub, green cells in Table 2) of the negative environmental impacts have been decreasing after the implementation of the RCP in the Russian Federation. The diagrams below (Fig. 12) show the percentage of cells marked with different colours in Table 2.

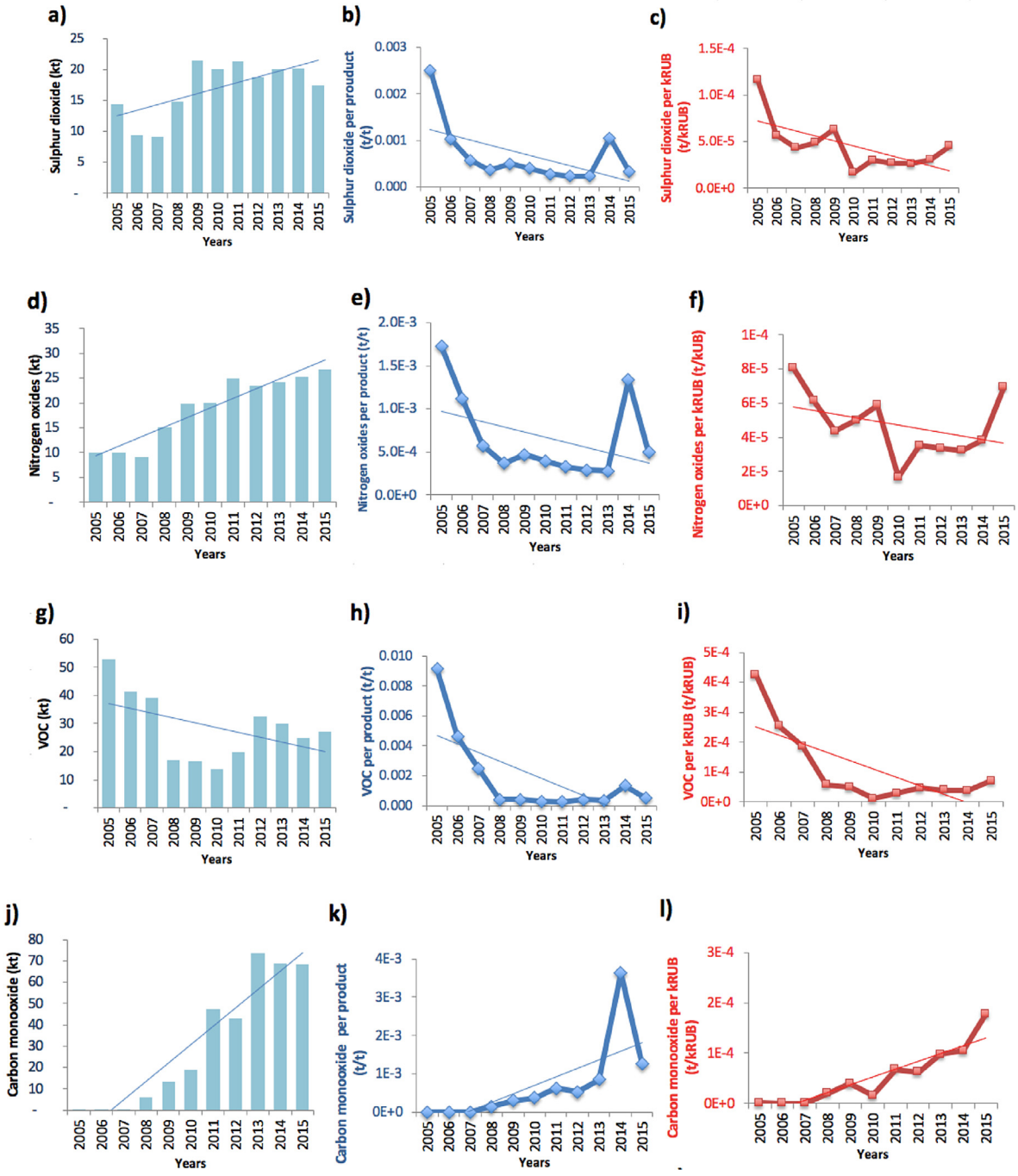


Fig. 5. Emissions of the main atmospheric pollutants, viz., SO_2, NO_x, VOC and CO of: a), d), g), and j) companies involved in the RCP (i_a, t); b), e), h), and k) companies involved in the RCP ($i_{norm,m}$, t/t product); c), f), i), and l) companies involved in the RCP ($i_{norm,\$}$, t/kRUB).

Fig. 12 shows a large percentage (about 50%) of the KPIs shows positive environmental aspects (green). It is assumed that the launch of the program has improved the environmental awareness of the companies, by proper encouragement and voluntary reporting regarding environmental performance. In detail, from 2005 to 2015, the SO_2 and VOC emissions showed a decreasing trend in the 11 y, indicating the reduction of atmospheric pollution. For soil pollution, the hazardous wastes for disposal have also been decreasing in the studies period. Regarding COD, nitrogen-containing compounds, and the total amount of hazardous compounds etc. discharged into the water systems have been reduced during the implementation of the program. While on the other hand, with an increase in total power and natural gas consumption, the CO_2 emission increased simultaneously during the period.

The last column in Table 2 provides the results of estimating trends for entire chemical industry sector in effluents, discharge, and disposed waste, which is determined based on the data provided from the annual reports from RF company involved in the RCP over a period of for years. Considering all companies involved in the RCP together manufacture approximately 30% of RF chemical products, and the data obtained allowed us to make predictive conclusions for the entire chemical industrial sector.

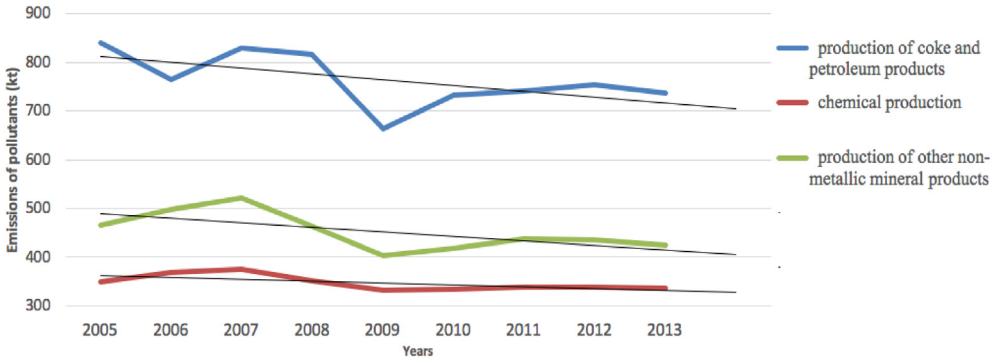


Fig. 6. Emissions of pollutants to the atmosphere from stationary sources.

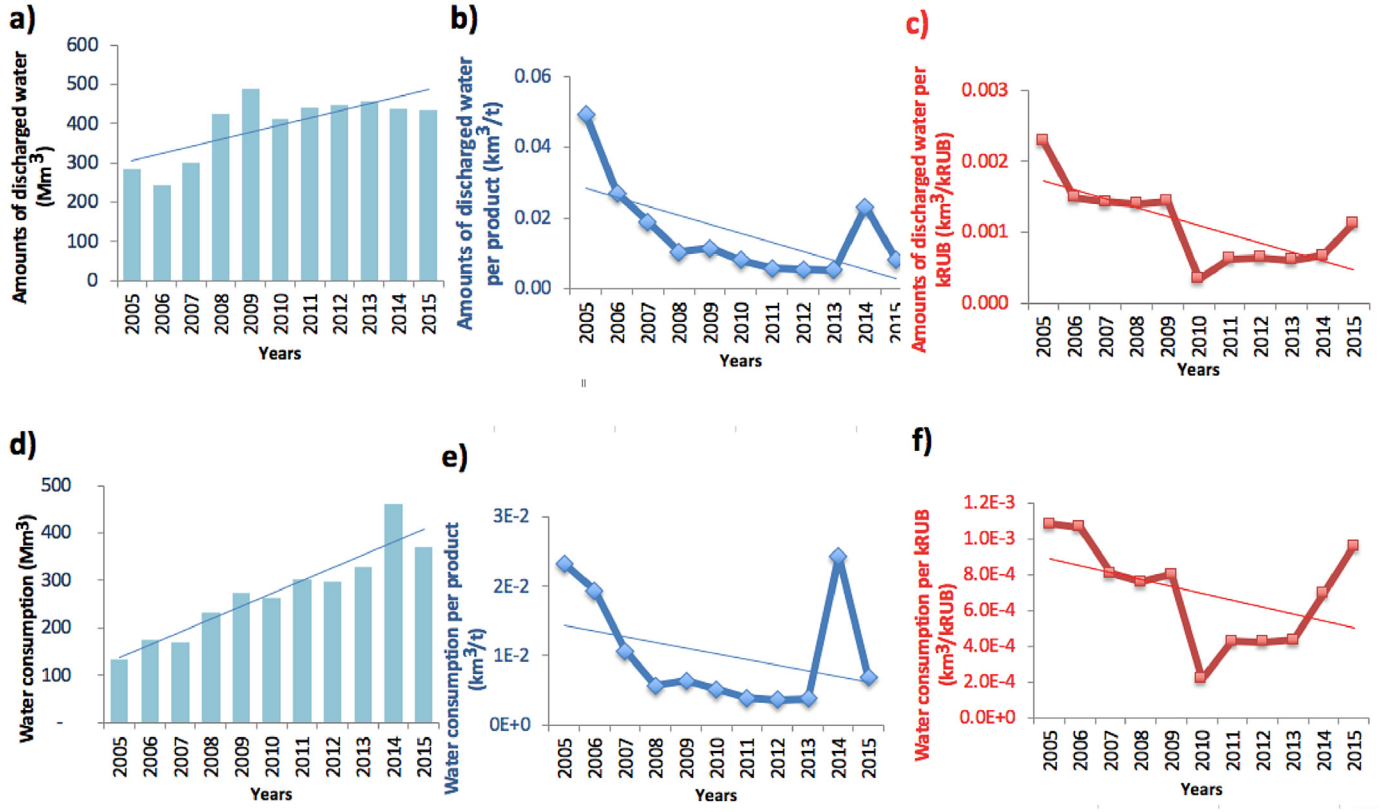


Fig. 7. Amount of consumed and discharged water by years: a) and d) Companies involved in the RCP (absolute value (i_a, t); b) and e) Companies involved in the RCP ($i_{norm,m}$, t/t product); c) and f) Companies involved in the RCP ($i_{norm,\$}$, t/kRUB).

But the emissions of CO, total direct CO^2 emissions, total GHG footprint, and energy consumption are increased in two or more cases (red colour in Table 2). These positions need the future work in the frame of the RCP. On the other parameters, there are no clear trends.

In Table 3 present the results for the efficiency of specific activities in which a decrease was observed. The economic efficiency of activity of chemical companies involved in RCP was estimated. The estimation of economic efficiency of activity of chemical companies involved in RCP was based on the generalised individual achievements with respect to the reduction of effluents, discharge, and disposed waste, which were calculated on stage 3 of the proposal the heuristic approximation algorithm. The resulting efficiency estimates were aggregated and compared to the data on expenses on environmental protection (see Table 3).

5.2. Comparison with other countries

In the 21st century, the RF chemical industries started to develop, and the production of chemical products also started to increase, which led to an increase in GHG emissions (Yang et al., 2017). The carbon emissions declined mostly because of the changes in industrial activities from 1992 to 2000, which accounted for 67.4% of the total CO_2 emissions (Rüstemoglu and Andrésb, 2016).

Fig. 13 showed that from 2005 to 2014, the CO_2 emissions of most CIS countries (e.g. Uzbekistan, Belarus, Azerbaijan, Georgia, and Tajikistan) have no major changes. CO_2 emissions of Ukraine showed slightly decreasing, while for Armenia is increasing at a considerable rate. For the RF, the overall trend of CO_2 emissions is increasing, while there is a remarkable drop from 2012 to 2014.

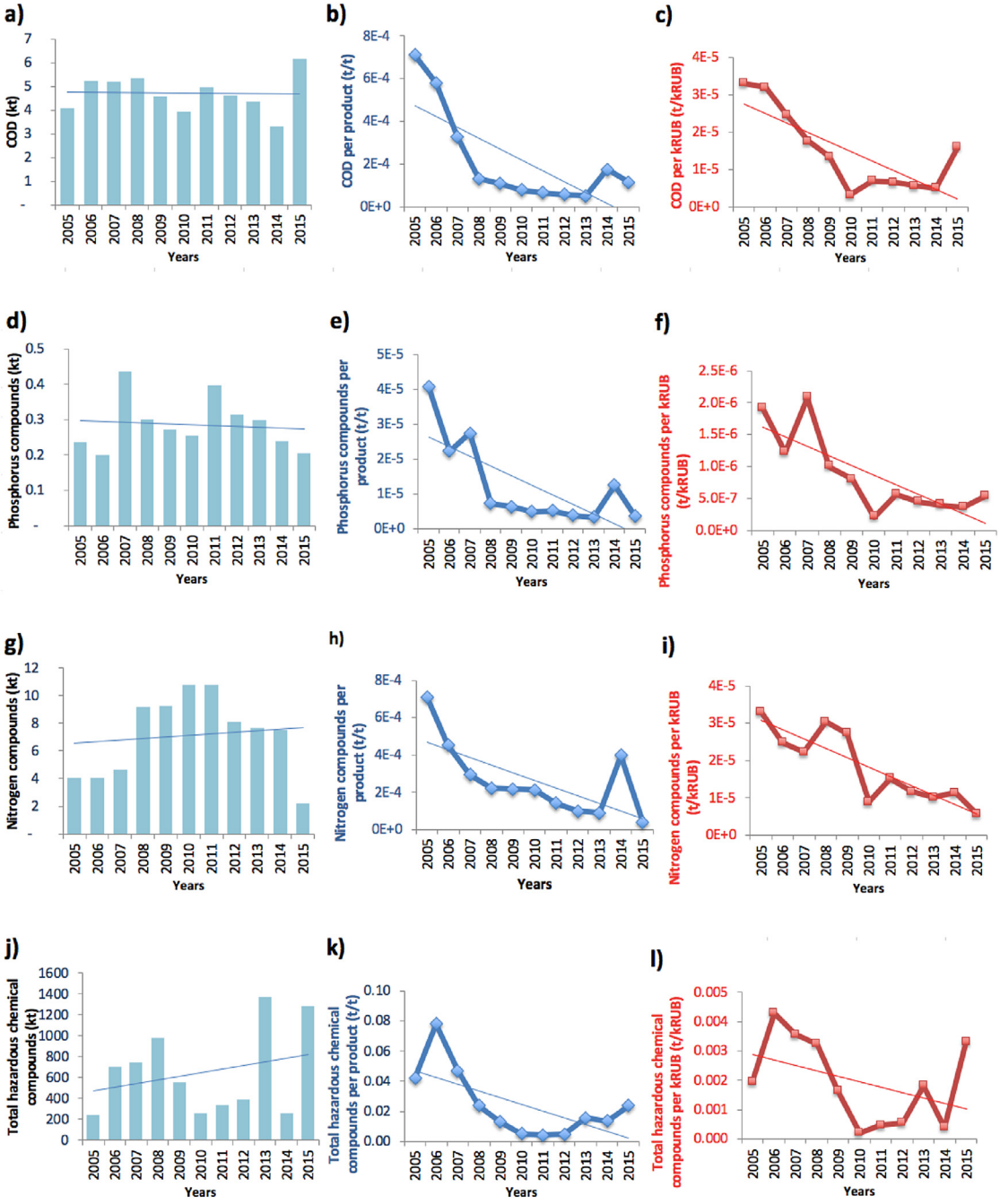


Fig. 8. Changes of the COD, of P– and N-containing chemical compounds and hazardous chemical compounds by years: a), d), g), and j) Companies involved in the RCP (i_a, t); b), e), h), and k) Companies involved in the RCP ($i_{norm,m}$, t/t product); c), f), i), and l) Companies involved in the RCP ($i_{norm,\$}$, t/kRUB).

It indicated that the implementation of the RCP has effectively affected the environmental performance of the chemical industries by improving the awareness of the impact of GHG emissions on climate changes. In addition, the government policy of the RF has paid great attention to the environmental issues since 2011, especially to the reduction of GHG emissions, which encourages the chemical enterprises for better performance on improving energy efficiency and reducing GHG emissions. The results also confirm the fact that better performance on environmental protection can be achieved when voluntary initiatives are supported by administrative decisions at a state level.

With the development of the information system, the concept of big data has been emerging. Based on big data, the concept of smart cities, smart industries, as well as climate-smart agriculture has been initiated and investigated (Saj et al., 2017). The development of big data would also facilitate the assessment and mitigation of environmental issues, including the GHG emissions, water scarcity, and degradation, as well as soil pollution, etc (Rathore et al., 2018). However, the utilizing of big data in practical policy-making is still being investigated. (Giest, 2017). Data incompletion has been one of the common issues for various larger-scale studies, and the assessment results in this study are also affected by the lack of data availability and quality. Since the report by the plants is completely voluntary, not all data of the reported periods were included in the

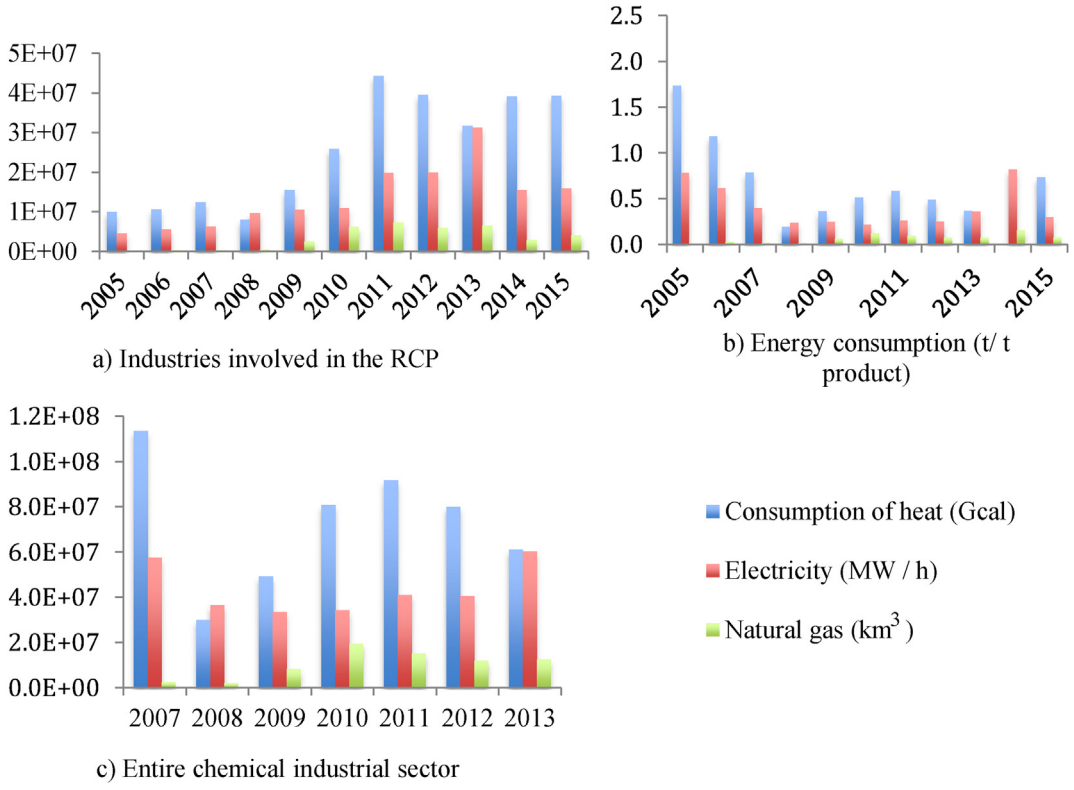


Fig. 9. Changes in the consumption of heat, electricity and natural gas: a) Companies involved in the RCP; b) Companies involved in the RCP (per t product); c) Entire chemical industrial sector.

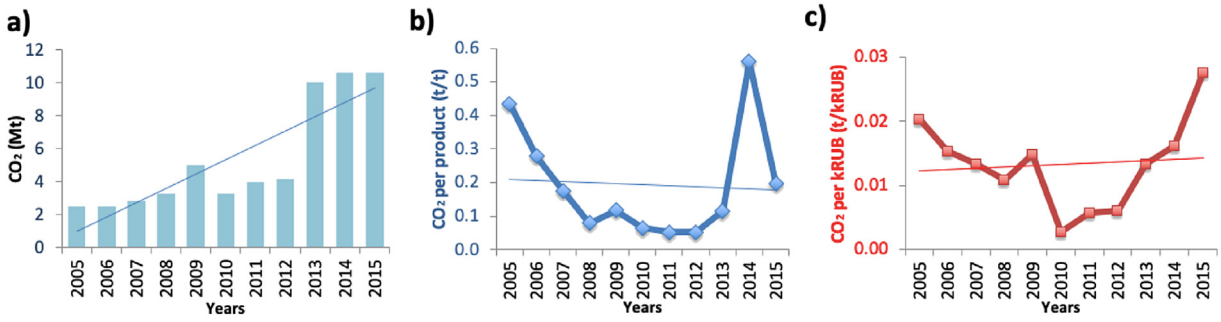


Fig. 10. Direct CO_2 emissions and GHG footprint in CO_2 equivalent: a) Companies involved in the RCP (i_a, t CO_{2eq}); b) Company involved in the RCP ($i_{norm,m}$, t CO_{2eq}/t product); c) Companies involved in the RCP ($i_{norm,\$}$, t CO_{2eq}/kRUB).

aggregated industry report. Some one-time reported data were provided by various small and medium-sized businesses, which did not make sufficient contribution to the aggregation of the whole industrial dataset. The companies providing these reports may have undergone renovation, opened new operations, revamped and/or enhanced their production capacities. Consequently, the inefficiency in data completion directly affects the reliability of the assessment and makes it difficult for direct analysis.

6. Conclusions

RCP focuses on management practices, rather than quantitative environmental targets which makes performance measurement difficult. The voluntary character of the reporting and the gaps in data provided by companies interfere considerably with the resulting figures (e.g. see CO absolute and relative indicators, Fig. 5) and make it difficult to consider them as accurate enough for rigorous quantitative analysis. It is obvious the collected data is insufficient for direct assessment, and more precise results can be reached by combining the approaches.

To tackle this issue, a heuristic approximation algorithm has been employed for the assessment of the environmental impact of the chemical industries. The algorithm has been based on using the large data set collected from the program reporting on the environmental KPIs of chemical enterprises involved in the RCP in the RF. The analysis has shown that the developed heuristic processing algorithm may further be used for the systematic analysis of the environmental impact indicators of the chemical companies. Dealing with the data incompletion, three different approaches were combined for the estimation:

1) Estimation based on the absolute value

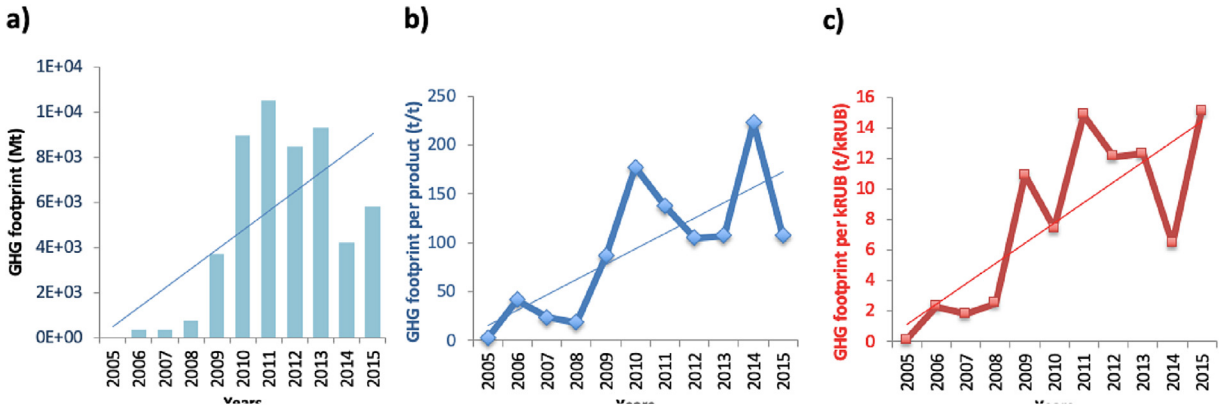


Fig. 11. Dynamics of GHG footprint of the companies involved in the RCP: a) Absolute value (i_a, t); b) footprint of unit product ($i_{norm,m}$, t/t product), and c) footprint of unit RUB ($i_{norm,\$}$, t/kRUB).

Table 2
Environmental impact indicators changing trend (Chemical industries involved in the RCP).

Indicators	Absolute value (i_a)	Relative indicators		With approximation of gaps	Trends for the entire chemical industrial sector
		t/product ($i_{norm,m}$)	t/kRUB ($i_{norm,\$}$)		
Soil Pollution					
Hazardous waste	Decrease	Decrease	Decrease	Decrease	Stable
Non-hazardous waste	No clear trend	Decrease	Decrease	Decrease	Decrease
Atmospheric pollution					
SO_2	Increase	Decrease	Decrease	Decrease	Decrease
NO_x	Increase	Decrease	Decrease	Increase	Decrease
VOC	Decrease	Decrease	Decrease	Decrease	Stable
CO	Increase	Increase	Increase	Increase	Increase
Water Consumption and Pollution					
Water discharge	Increase	Decrease	Decrease	Decrease	Decrease
Water consumption	Increase	Decrease	No clear trend	Decrease	Decrease
COD	Stable	Decrease	Decrease	Decrease	Decrease
P-containing compounds	Stable	Decrease	Decrease	Increase	Stable
N-containing compounds	No clear trend	Decrease	Decrease	Decrease	Decrease
Hazardous chemical compounds	No clear trend	Decrease	No clear trend	Decrease	Decrease
Energy consumption					
Heat	Increase	Decrease	Decrease	Increase	No clear trend
Electricity	Increase	No clear trend	No clear trend	Increase	No clear trend
Natural Gas	Increase	Increase	Increase	Increase	Increase
Total energy[a]	Increase	No clear trend	No clear trend	Increase	No clear trend
Climate Change					
Total GHG direct emissions	Increase	No clear trend	No clear trend	Increase	No clear trend
GHG footprint (total direct + indirect emission)	No clear trend	Increase	Increase	N/A	No clear trend

[a] Total energy usage is the sum of the consumption of fossil fuels, purchase of energy and self-produced energy.

2) The values are standardized on 1 t of products and/or k RUB
3) Extrapolation and interpolation methods are used to replenish the missing data collected from enterprises.

With the voluntary reporting dataset, the environmental performance of the industries involved in the Responsible Care Program (RCP) is assessed. The results showed that during the study

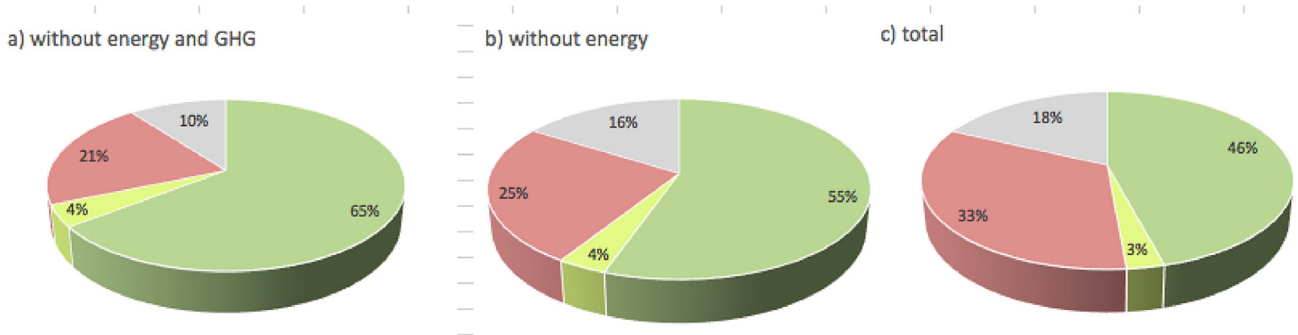


Fig. 12. Percentage of different trends of the KPIs describing the environmental impact; a) without KPIs characterisation of energy consumption and GHG; b) without taking into account the energy KPIs; c) for the all KPIs in total.

Table 3
System analysis results for the efficiency of environmental protection activities of RF chemical company.

Indicators	The efficiency of environmental protection for a company involved in RCP in the 11 y period	
	per kRUB of environment protection Investment	per kRUB of atmospheric air protection Investment
Hazardous waste	$9*10^{-3}$ t/kRUB	N/A
Non-hazardous waste	0.01 t/kRUB	N/A
SO_2	$4*10^{-6}$ t/kRUB	$4*10^{-5}$ t/kRUB
VOC	$9*10^{-3}$ t/kRUB	0.02 t/kRUB
Water discharge	$7*10^{-4}$ m^3/RUB	N/A
COD	$2*10^{-5}$ t/kRUB	N/A
N-containing compounds	$4*10^{-5}$ t/kRUB	N/A
Hazardous chemical compounds	$3*10^{-3}$ t/kRUB	N/A

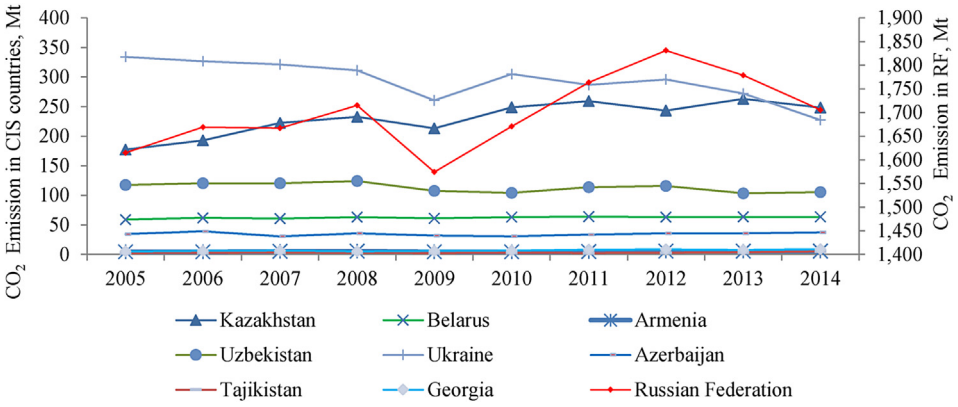


Fig. 13. Comparison of CO_2 emission of different countries from 2005 to 2014.

period, most of the assessed indicators for soil pollution and water system pollution showed a trend of decreasing. From 2005 to 2015, the specific hazardous and non-hazardous waste disposal decreased from 0.5 t/t product and 16 t/kRUB to less than 0.002 t/product and 2 t/kRUB. The total water consumption is increasing but the specific water consumption has been reduced from 25 m^3/t product to less than 8 m^3/t product, which indicates an increase of water use efficiency. The specific energy consumption, including heat and natural gas, reached a peak in 2011 and keep decreasing in the following years. At the same time, the specific electricity increased from 2005 to 2015. The total GHG emissions of the industries involved in the RCP increased from 2.8 Mt CO_{2eq} to 10 Mt CO_{2eq}, but the unit product GHG emissions decreased from 0.45 t CO_{2eq}/t to 0.2 t CO_{2eq}/t.

It's necessary to note that from 1992 to 2000, the effect of economic activities effect has experienced a reducing impact in the RF's overall CO_2 emissions, and there was a considerable decline in GHG emissions in this period. However, the energy intensity successfully offsets this increasing impact of economic activity, and it can be seen as a result in the presented investigation. From 2011 to 2015, the increase in GHG emissions has been mitigated and reached a relatively steady state. A primary conclusion is that the environmental impact with short-term visible results (e.g. soil pollution and water pollution) have been reduced significantly, while the focus of environmental impact such as GHG emissions, which does not have visible impact in short term, has not been paid enough attention.

The methodology might prove beneficial for trend analysis, especially if more data consistency is achieved (by using additional statistical data, data processing, more companies joining RCP and providing consistent data, etc). In the framework of further research on this topic is intended to use the additional data for 2016 and 2017, and computational error can also be reduced for better estimation. As the authors are planning to clarify some gaps in the information having sent the corresponding inquiries to the enterprises. These actions would allow evaluating the effectiveness of the proposed algorithm. It is also expected that this algorithm can be applied and for processing the reports from other countries.

Acknowledgements

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Nomenclature

J	The number of chemical companies
i_a^n	Aggregated absolute indicators
n	The reporting year
a	The type of the environmental impacts including Solid waste (hazardous and non-hazardous); Atmospheric pollutants (SO_2, VOC, NOx, CO); GHGs emissions (CO_2, NOx, HFCs, and CH_4, Water pollutant (Water consumption and discharge, COD, phosphorus-/nitrogen-containing compounds, and discharged hazardous chemical compounds); Energy consumption (Electricity, heat, natural gas consumption)
V_m^n	Chemical products, t
$V_\$^n$	Volume of manufactured products in monetary terms, RUB
$i_{inorm,m}^{n,i}$	Normalised aggregated indicators t/t product

$i^{n,i}_{norm,\$}$	Normalised aggregated indicators, t/RUB
E^i_j	The slope of the trend line of the KPI
E^i_{mean}	The averaged performance parameter for the all chemical companies involved in the RCP for the KPI
$i^{n,i}_{ind,m}$	Aggregated absolute indicators for entire chemical industry with using the normalised aggregated indicators ($i^{n,i}_{inorm,m}$)
$V^n_{ind,m}$	Chemical products of entire chemical industry, t
$i^{n,i}_{ind,\$}$	Aggregated absolute indicators for entire chemical industry with using the normalised aggregated indicators ($i^{n,i}_{inorm,\$}$)
$V^n_{ind,\$}$	Unit of RUB in mass terms of entire chemical industry, RUB
E^i_{total}	Performance parameter for the all chemical companies involved in the RCP for the KPI
E^i_{mean}	The efficiency of environmental activities of a chemical company involved in the RCP
S^n_j	Total environmental protection expense of the *j*th particular company for the *n*th y, RUB
$S^n_{atm,j}$	Total atmospheric air protection expense of *j*th particular company for the *n*th y, RUB
E	annual CO_2 emissions in weight units, t/y
M	actual fuel consumption for the year, t/y
K_1	carbon oxidation factor of the fuel
NCV	net calorific value, J/t
K_2	C emission factor, t/J
V	The volume of natural gas, m^3

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